Machine learning and multi-scale modeling

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Modern machine learning has had remarkable success in all kinds of AI applications, and is also poised to change fundamentally the way we do physical modeling. In this talk, I will give an overview on some of the theoretical and practical issues that I consider most important in this exciting area.

The first part of this talk will be focused on the following question: How can we make use of modern machine learning tools to help build reliable and practical physical models?

Here we will address two issues (mostly using the example of molecular dynamics):
(1) building machine learning models that satisfy physical constraints;
(2) using microscopic models to generate the optimal data set.

The second part of the talk will be devoted to some of the theoretical issues. Serious difficulties arise due to the fact that the underlying dimensionality is high, the neural network models are non-convex and highly over-parametrized. We don't yet have a complete mathematical picture about neural network-based machine learning but we will discuss the current status. Specifically, we will discuss the representation of high dimensional functions, optimal a priori estimates of the generalization error for neural networks, and gradient decent dynamics.